



# Elastic properties of a single-walled carbon nanotube under a thermal environment



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## ABSTRACT

In this paper, a temperature-dependent and thickness-independent molecular structure mechanics model is established to study the elastic properties of single-walled carbon nanotubes (SWNTs) under a thermal environment. A linear coefficient of thermal (LCTE), which changes continuously with the temperature, is also adopted. The Young's modulus and the Poisson's ratio of SWNTs for different temperatures are analyzed. It is found that the Young's moduli of both armchair and zigzag SWNTs decrease with the increase of the temperature, but the Poisson's ratio is not dependent on the temperature. Moreover, it is noted that for a given nanotube diameter, the Young's moduli of armchair nanotubes are larger than those for zigzag nanotubes slightly. However, for a given temperature the Young's moduli of both armchair and zigzag nanotubes increase with increasing nanotube diameters.

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## 1. Introduction

Since their discovery in 1991 [1], carbon nanotubes (CNTs) have been widely perceived as a very promising material for applications in nano-engineering due to their exceptional mechanical and electronic properties. For example, experimental investigations and numerical simulations have shown that carbon nanotubes have Young's modulus on the order of TPa [2,3], with potential applications in ultra-strong composite materials [4,5], nano-mechanical and nano-electro devices. It is widely accepted that many nano-electronics may undergo high temperature when they were manufactured and operating. It has been shown that the postbuckling behavior of SWNTs subjected to axial compression depends on temperature [6,7]. Therefore, establishing a theory to study the thermal mechanical properties of CNTs is very important for their practical engineering applications.

However, due to the challenge in nanoscale experiments and modeling, the experiments studying on the CTE of CNTs are very limited. To study the CNT properties in thermal environment, one way is the molecular dynamics (MD) [8–10]. Although limited studies have been down in this way in the thermal environment about CNT, it is generally recognized that it is accurate in result. Nachiket et al. [8] investigated the coefficient of thermal expansion (CTE) of (5,5) and (10,10) armchair CNTs, and found that the CTE of the CNT in the direction of axial was higher than that in the radial

direction. It was noted that the CTE is associated with the change in C–C bond length,  $\alpha_{C-C} = 7.1 \pm 0.2 \times 10^{-6}/K$ . However, there is only a single value of the CTE in the axial direction, and another fixed value corresponding to the direction of radial was reported. There is no dependence being founded between the CTE of SWNT and temperature, that is contrary to the results [9–12]. Kwon et al. [9] performed molecular dynamics simulations to study shape changes of carbon fullerenes and nanotubes with increasing temperature, and the curve for the LCTE of the (10,10) armchair CNT changed with temperatures was given. Maniwa et al. [12] focus on the CTE of SWNT and CNT bundles, and a strong temperature dependence of CTEs was represented.

However, due to the finite ability of Modern calculating devices, the simulation of larger systems over long time must be left to continuum mechanics methods. There are two types of continuum mechanics studying the elastic properties of CNTs with temperatures. One is to model a CNT as a linear elastic thin shell [13–16] and single value of the CTE in the axial and radical directions was adopted. Generally,  $\alpha_1 = -1.6 \times 10^{-6}$ ,  $\alpha_2 = -0.5 \times 10^{-6}$  at low and room temperature,  $\alpha_1 = 1.1 \times 10^{-6}$ ,  $\alpha_2 = 0.8 \times 10^{-6}$  at high temperature, where  $\alpha_1$  and  $\alpha_2$  are the CTEs of CNTs in the axial and circumferential directions, respectively. This way was first performed by Yao et al. [13] and widely accepted by many researchers [14–16], quickly. However, such a linear elastic shell theory cannot account for the important effect of CNT chirality (e.g., armchair and zig-zag chiral CNTs) on their mechanical behavior. It also does not take the nonlinear, multi-body atomistic interactions characterized by the interatomic potential [17,18] into consideration, which is

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inevitably affected by the carbon nanotube thickness and is not clearly defined till now. Another type of continuum study on CNTs is to take into account the nonlinear, multi-body interatomic potential of carbon for the continuum analysis [19–21], directly, via the Cauchy–Born rule [22]. Based on the results of Zhang et al. [19,20], in which the Helmholtz free energy is introduced, Jiang et al. [23] take the finite temperature into consideration, successfully. Based on the results of Jiang et al. [23], an elastic property and temperature dependent model of SWNTs has been established by Wang and Guo [24] via a so-called higher order Cauchy–Born rule [21]. But the theoretical researches about the elastic properties of CNTs on the thermal environment via the molecular mechanics are still not well constructed at present. To our best knowledge, Zhu et al. [25] is the only one who has established a temperature-dependent model about SWNTs based on the molecular mechanics. They have established the proportional relationship between the  $K_p$ ,  $K_\theta$  and the temperature  $T$ , where the  $K_p$ ,  $K_\theta$  is the stretching force constant of C–C bond and the bending force constant between two adjacent bonds, respectively. But they are still not avoiding the impact of the SWNT thickness which is not well defined till now. As the very limited literatures about the CTE of SWNT can be applied, the CTE they used in their research is directly coming from the simulated results of C<sub>60</sub>. Therefore, the results obtained are not accurate enough to predict the elastic properties of the SWNT on the thermal environment. A size-dependent analytical model [26] is presented to relate the elastic properties of a SWNT to its atomic structure based on a molecular mechanics approach and a modified Morse model [27]. A very simple thickness-independent model is presented by Natsuki and Endo [28] based on the molecular mechanics. However, it is worth noting that both of the above thickness-independent models for SCNTs are established without considering the thermal effect.

It is widely recognized that in practical nano-engineering applications, CNTs and CNTs based nanoscale devices often work in thermal environments. Therefore, it is very important to propose a model that can be used to predict the thermo-mechanical properties of CNTs at different temperatures easily. However, a few research works on this topic can be found in the literatures. This paper plans to present a simply and efficiently computational approach to investigate the effect of environmental temperature on the elastic properties of SWNTs and to avoid the impact of tube thickness in the same time. In the present study, therefore, a thickness-independent and temperature-dependent molecular structure mechanics model of SWNT under the thermal environment is proposed to study the elastic properties of SWNT at different temperatures based on the molecular mechanics. A continuous LCTE for the armchair tube (10,10) is also adopted as the CTE of C–C bonds to analyze the elastic properties of SWNT qualitatively.

## 2. Structure of carbon nanotubes

A SWNT is formed by rolling a single graphene sheet to form a hollow tube composed of carbon hexagons. Fig. 1 shows a segment of a hexagonal graphene sheet. The fundamental CNTs can be classified into three categories of zigzag, armchair and arbitrary chiral tubes in terms of the chiral vector integers ( $n, m$ ). The symmetry groups of carbon nanotubes are represented by the armchair nanotube ( $n = m$ ) and zigzag nanotube ( $m = 0$ ), and the rolling directions of armchair and zigzag CNT are denoted by blue arrows, as shown in Fig. 1. The truss model for the single-walled carbon nanotube in a thermal environment, which is denoted by  $T$ , is shown in Fig. 2, in which the covalent chemical bonds are treated as connecting elements between two carbon atoms [7].

In Fig. 2, the molecular structure mechanics model is substituted with a frame structure model in order to form an equivalent-continuum model. Parameter  $\theta$  is the angle between bond  $IJ$  and bond  $JK$  in room temperature. Here,  $K_p^T$ , and  $C_\theta^T$  are the stretching and bending force constants associated with the C–C bonds length  $b$  (e.g.,  $I–J$  and  $J–K$ ) and angle variance  $\theta$  in different environment temperatures, respectively, and  $T$  denotes an environment temperature of the frame structure model. The spring elements which represent the  $K_p^T$  and  $C_\theta^T$  are used for modeling the axial deformation of the carbon-to-carbon bond and the angular distortion of the bond angles. Subsequently, the temperature-dependent stretching force and twisting moment acting on the element of the frame structure can be written as

$$F = K_p^T \Delta b, \quad (1a)$$

$$M = C_\theta^T \Delta \theta, \quad (1b)$$

where  $\Delta b$  and  $\Delta \theta$  are the elongation and angle variation, respectively.

For establishing a thickness-independent model of single-walled carbon nanotubes accounting for the effect of the environmental temperature, we first establish the temperature-dependent relationships about  $K_p^T$ ,  $C_\theta^T$  and  $b^T$  through the C–C bonds CTE  $\alpha_{C-C}$  defined [8], from which a temperature-dependent and thickness-independent model can be established based on the study [26].

## 3. Temperature-dependent force fields

The potential energy of an arbitrary molecule structure is the total system potential energy,  $E$ , which can be expressed as a sum of several individual energy terms [29] as follows:

$$E = \Sigma E_R + \Sigma E_\theta + \Sigma E_\tau + \Sigma E_{\omega} + \Sigma E_{vdW} + \Sigma E_{es}, \quad (2)$$

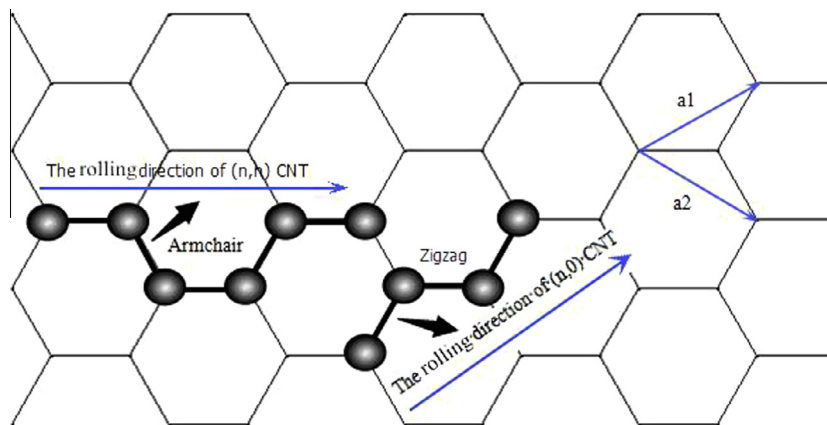


Fig. 1. Schematic illustration of a hexagonal graphene sheet.

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